



chain nodes :

1 2 3 4 5 51 52 54 55

ring nodes :

6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30
31 32 33 38 39 40 41 42 43 44 45 46 47

chain bonds :

1-2 2-3 3-4 3-5 5-51 51-55 52-54 52-55

ring bonds :

6-7 6-11 7-8 8-9 9-10 10-11 10-12 11-15 12-13 13-14 14-15 16-17 16-21 17-18 18-19
19-20 20-21 22-23 22-27 23-24 24-25 25-26 26-27 28-29 28-33 29-30 30-31 31-32
32-33 38-39 38-43 39-40 40-41 41-42 42-43 42-44 43-47 44-45 45-46 46-47

exact/norm bonds :

1-2 2-3 3-4 3-5 5-51 51-55 52-54 52-55

normalized bonds :

6-7 6-11 7-8 8-9 9-10 10-11 10-12 11-15 12-13 13-14 14-15 16-17 16-21 17-18 18-19
19-20 20-21 22-23 22-27 23-24 24-25 25-26 26-27 28-29 28-33 29-30 30-31 31-32
32-33 38-39 38-43 39-40 40-41 41-42 42-43 42-44 43-47 44-45 45-46 46-47

isolated ring systems :

containing 6 : 16 : 22 : 28 : 38 :

G1:[*1], [*2], [*3], [*4], [*5]

Match level :

1:Atom 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom
22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom
32:Atom 33:Atom 38:Atom 39:Atom 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom 45:Atom
46:Atom 47:Atom 51:CLASS 52:Atom 54:CLASS 55:CLASS

Generic attributes :

52:

Saturation : Unsaturated

Number of Carbon Atoms : less than 7

Number of Hetero Atoms : Exactly 1

Type of Ring System : Monocyclic

Element Count :
Node 52: Limited
C,C5
N,N1